Atomic scale design of nanostructures

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Recent advances in theoretical methods and high performance computing allow for reliable first-principles predictions of complex nanostructured materials and devices. This talk will discuss three examples: (i) Nanotube-cluster systems, which behave as effective chemical sensors whose electrical response changes dramatically upon adsorption of small molecules onto the metal clusters. (ii) Polarization and piezoelectric properties of BN nanotubes and BN-based polymers. We show that BN nanotubes are excellent nano piezoelectrics that could form the core of high-performance actuators and sensors, but have no spontaneous polarization. However, the predicted polymers offer 100% improvement in both ferro and piezoelectricity over those in current use. (iii) We demonstrate that reflectance anisotropy of a semiconductor surface or interface provides a *unique* signature of its atomic structure. The corresponding line-shape can be obtained from first-principles calculations, leading to *unambiguous* identification of the structure and potentially enabling feedback-controlled growth of device structures with nearly monolayer resolution. A number of applications to III-V and Si surfaces will be discussed.

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